Notes on Gaussian Quadrature

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Introduction

Gaussian quadrature is particularly efficient for integrating polynomials and uses specially chosen points and weights to achieve high accuracy.

Brief Overview

Gaussian quadrature approximates this integral using:

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

where x_i are the nodes and w_i are the weights. The nodes and weights are chosen such that the method is exact for polynomials of degree $2n-1$ or lower. Typically, this integral is from $[-1, 1]$.

Motivation

Our intuition comes from the trapezoid rule, which only provide exact solutions to integrals for linear functions. But we can do better, take n nodes $x_1, x_2, \cdots, x_n$. We can improve the trapezoid by choosing the weights such that they are exact for linear, quadratic, cubic, up to polynomials of degree $n-1$.

$$\int_{-1}^{1} f \approx w_1 f(x_1) + w_2 f(x_2) + \cdots + w_n f(x_n) \tag{1}$$

$$\begin{aligned}
f(x) = 1 \to \int_{-1}^{1} 1\,dx = 2 = w_1 + w_2 + \cdot + w_n \\
f(x) = x \to \int_{-1}^{1} x\,dx = 0 = w_1 x_1 + w_2 x_2 + \cdot + w_n x_n \\
\vdots \\
f(x) = x^{n-1} \to \int_{-1}^{1} x^{n-1}\,dx = 0 = w_1 x_1^{n-1} + w_2 x_2^{n-1} + \cdots + w_n x_n^{n-1}
\end{aligned}$$

Resulting in the following linear equation (with a Vandermonde Matrix):

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & \ddots & \cdots & x_n \\ \vdots & & \ddots & \\ x_1^{n-1} & x_2^{n-1} & \cdots & x_n^{n-1} \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ \vdots \\ b_i \end{bmatrix}$$

In practice, this method is not feasible because Vandermonde matrices are badly ill-conditioned, as the condition number increases exponentially, (https://arxiv.org/abs/1504.02118), resulting in slight changes in b causing large changes in w_i's.

Linear Algebra Intuition

Ultimately, this problem boils down to a linear algebra problem, and will require using polynomials as vectors, inner products, Gram-Schmidt orthogonalization. This arises because the integral is a linear operator.

Overview of Legendre Polynomials

Starting with the following basis and inner product:

$$\{1, x, x^2, \cdots, x^n\} \qquad \langle p, q \rangle = \int_{-1}^{1} p(x)q(x)\,dx$$

Performing the Gram-Schmidt process, we get the following orthogonal polynomials known as **Legendre Polynomials**.

$$\begin{aligned} L_0(x) =& 1 \\ L_1(x) =& x \\ L_2(x) =& \frac{1}{2}(3x^2 - 1) \\ & \vdots \end{aligned}$$

Note: they have been scaled such that $L_n(1) = 1$.
It is important to notice that $L_i(x)$ is orthogonal to all polynomials of degree less than i, meaning $\forall p \in \mathcal{P}$, $\langle L_i, p \rangle = 0$ for $\deg(p) \leq i$. Another important note is that they have exactly n roots over $\mathbb{R}$.

Developing Gaussian Quadrature

Given a polynomial of degree $2n-1$, namely $p(x)$, we can divide it by L_n, resulting in the following division with degrees:

$$\overbrace{p(x)}^{2n-1} = \overbrace{q(x)}^{n-1}\overbrace{L_n(x)}^{n} + \overbrace{r(x)}^{n-1} \tag{2}$$

Integrating both sides we get

$$\int_{-1}^{1} p(x)\,dx = \int_{-1}^{1} q(x)L_n(x)\,dx + \int_{-1}^{1} r(x)\,dx = 0 + \int_{-1}^{1} r(x)\,dx$$

because the orthogonality of $L_n(x)$.
Going back to quadrature, we can ensure the same behavior by picking nodes at the zeros of $L_n(x)$.
Because $\int_{-1}^{1} p(x)\,dx = \int_{-1}^{1} r(x)\,dx$, we can interpolate $r(x)$ exactly with Lagrange polynomials, resulting in

$$\int_{-1}^{1} r(x)\,dx = \int_{-1}^{1} \left(\sum_{i=1}^{n} f(x_i) l_i(x) \right) dx = \sum_{i=1}^{n} f(x_i) \int_{-1}^{1} l_i(x)\,dx$$

meaning we choose our weights the be the integral of the Lagrange basis polynomials, or

$$w_i = \int_{-1}^{1} \prod_{j=1 j \neq i}^{n} \frac{x - x_j}{x_i - x_j}\,dx$$

This results perfect interpolation of polynomials of degree $2n-1$, with n nodes. We can actually relate Lagrange and Legendre polynomials and then use the Christoffel-Darboux formula to rewrite the definition of the weights as

$$w_i = \frac{2}{(1 - x_i^2)(L_n'(x_i))^2} \tag{3}$$

Note on the Bounds

One must change an integral over $[a, b]$ to one over $[-1, 1]$ before using Gaussian Quadrature. This can be done with

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{b-a}{2} x + \frac{a+b}{2} \right) \frac{b-a}{2}\,dx$$

Resulting in a formula of:

$$\int_a^b f(x) \approx \frac{b-a}{2} \sum_{i=1}^{n} w_i f\left(\frac{b-a}{2} x_i + \frac{a+b}{2} \right) \tag{4}$$

Error estimate pg22. (https://www.math.umd.edu/ mariakc/AMSC466/LectureNotes/quadrature.p